

Generating Emissions Fields for WRF-Chem with PREP-CHEM-SRC

Rafael Santos Lima, Marcelo Alonso, Megan Bela,
Valter Oliveira, Rafael Fonseca, Madeleine Gácita, Gabriel Pereira,
Karla M. Longo, Saulo R. Freitas, Georg Grell

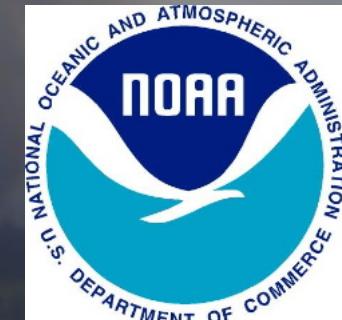
megan.bela@colorado.edu

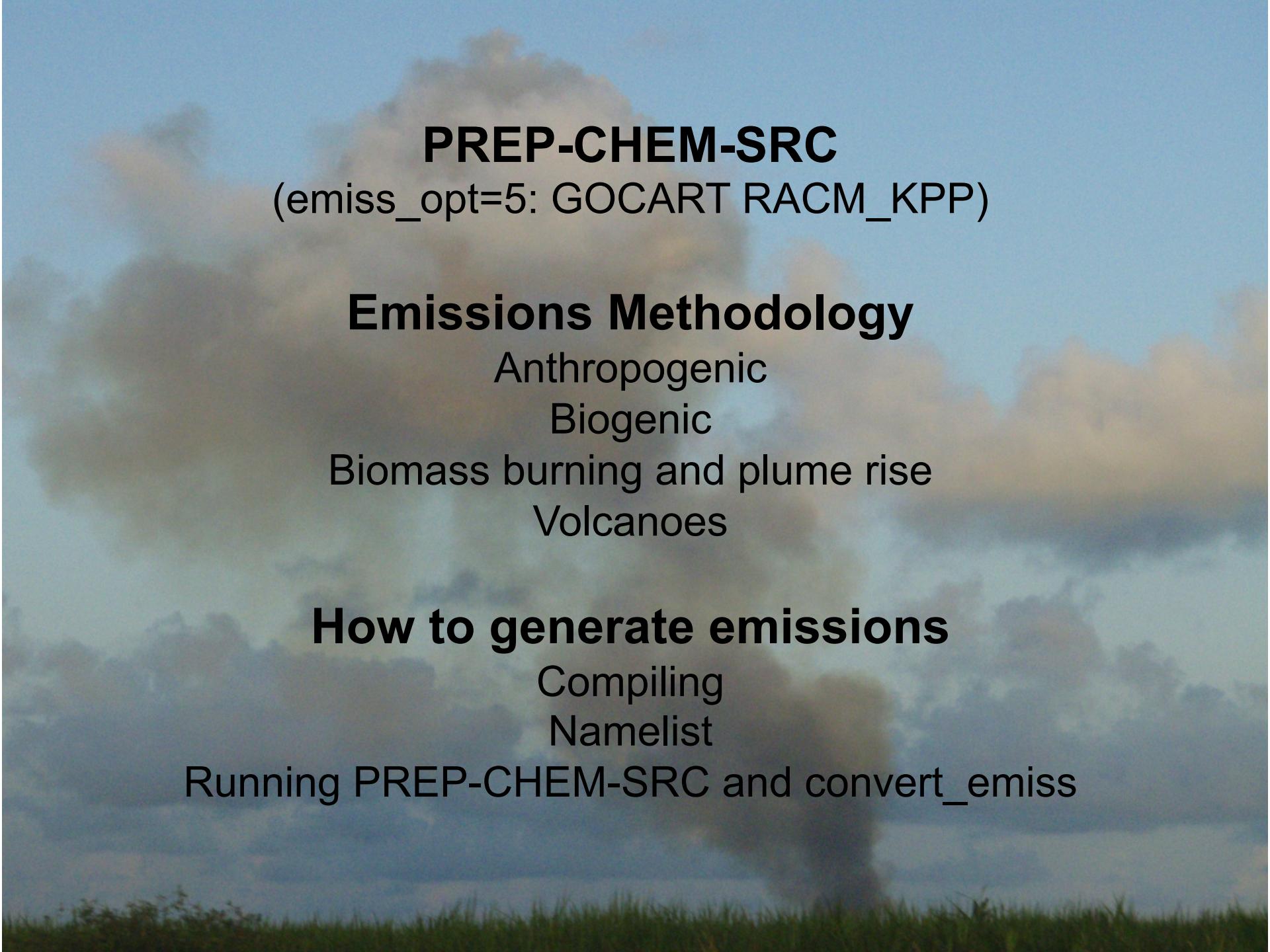
gmai@cptec.inpe.br

meioambiente.cptec.inpe.br



WRF-Chem Tutorial, July 25 2012
NCAR Foothills Laboratory, Boulder, CO





PREP-CHEM-SRC

(emiss_opt=5: GOCART RACM_KPP)

Emissions Methodology

Anthropogenic

Biogenic

Biomass burning and plume rise

Volcanoes

How to generate emissions

Compiling

Namelist

Running PREP-CHEM-SRC and convert_emiss

Anthropogenic emissions

Global Inventories

RETRO ($0.5^{\circ} \times 0.5^{\circ}$, monthly, 1960-2000)

GOCART

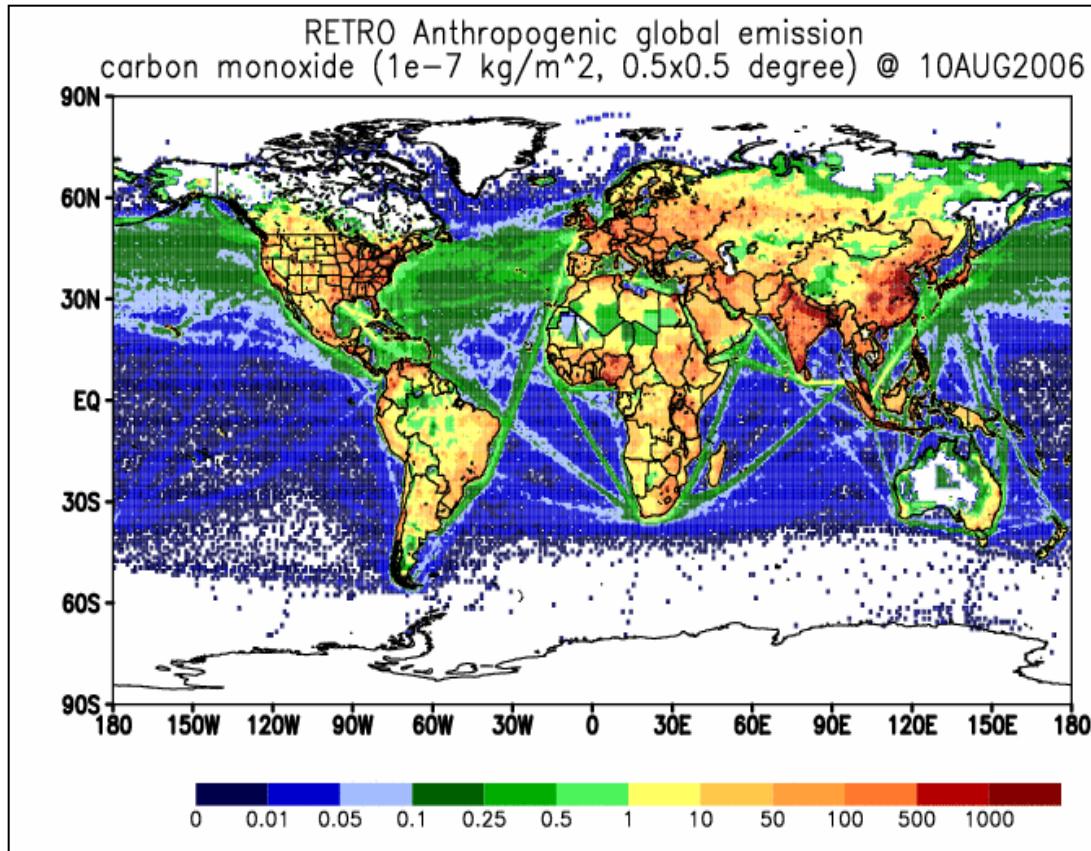
OC, BC and SO_2 ($1^{\circ} \times 1^{\circ}$, annual, 2006)

EDGAR v4.2 ($0.1^{\circ} \times 0.1^{\circ}$, annual, 1970-2008)

DMS ($1^{\circ} \times 1.25^{\circ}$, monthly)

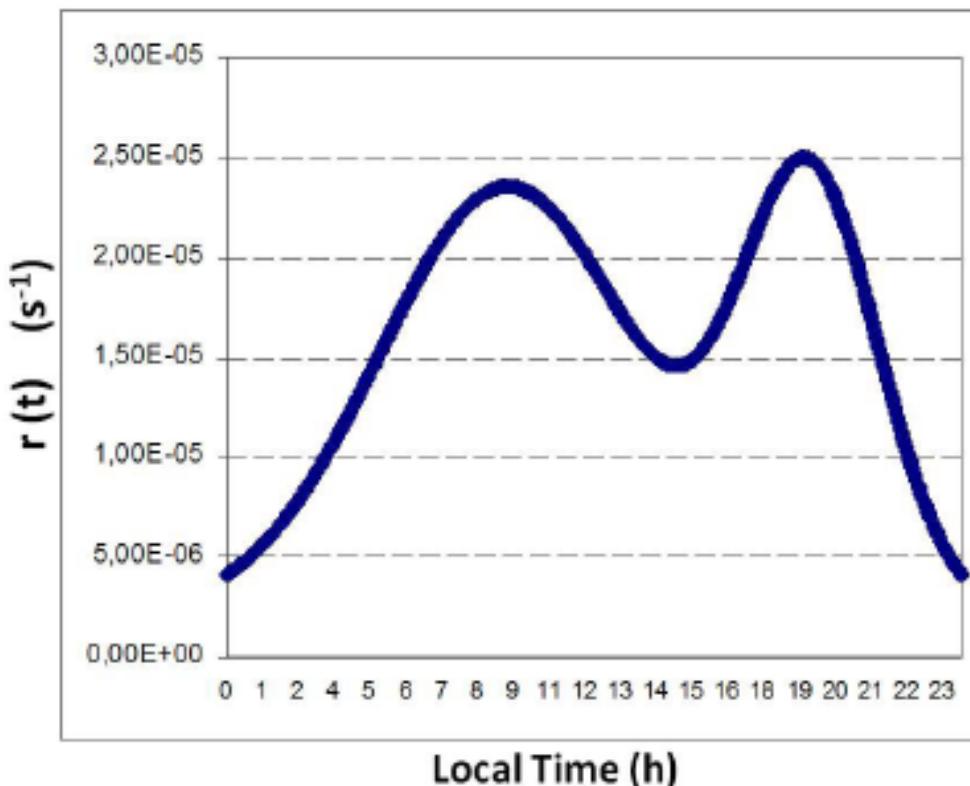
CO_2 , CH_4 , N_2O , HFCs, PFCs, SF_6

NO_3 , H_2O_2 and OH (3D, $1^{\circ} \times 1.25^{\circ}$ monthly, 2006)



Anthropogenic emissions

Diurnal cycle is applied inside WRF

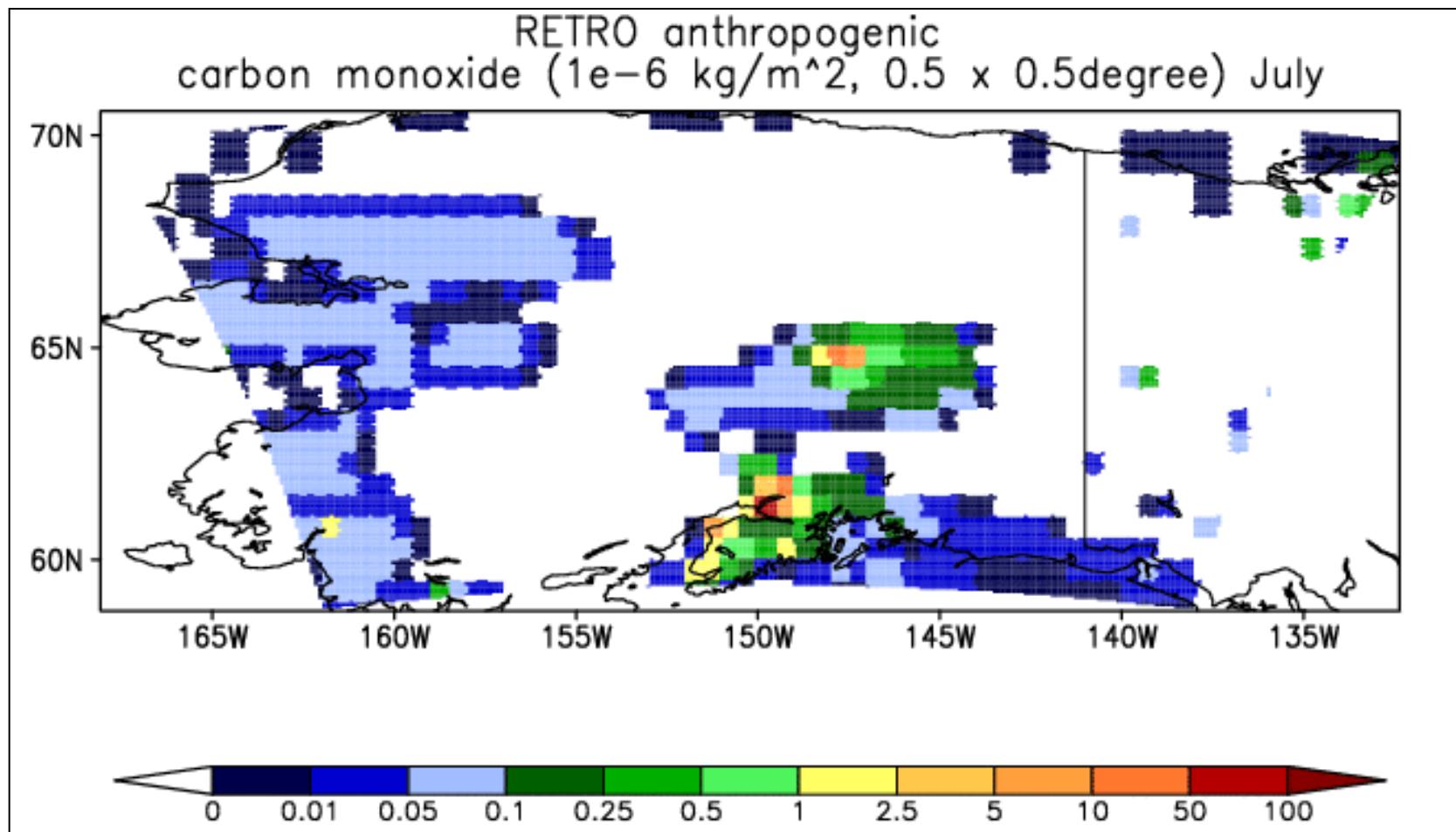


$$\int_0^{86400} r(t) dt = 1,$$

$$\bar{E}_\eta(k, t) = \begin{cases} \frac{F_\eta}{\bar{\rho}(k_1) \Delta z_1} r(t), & k = 1 \text{ (surface)} \\ 0, & k > 1 \text{ (above)} \end{cases},$$

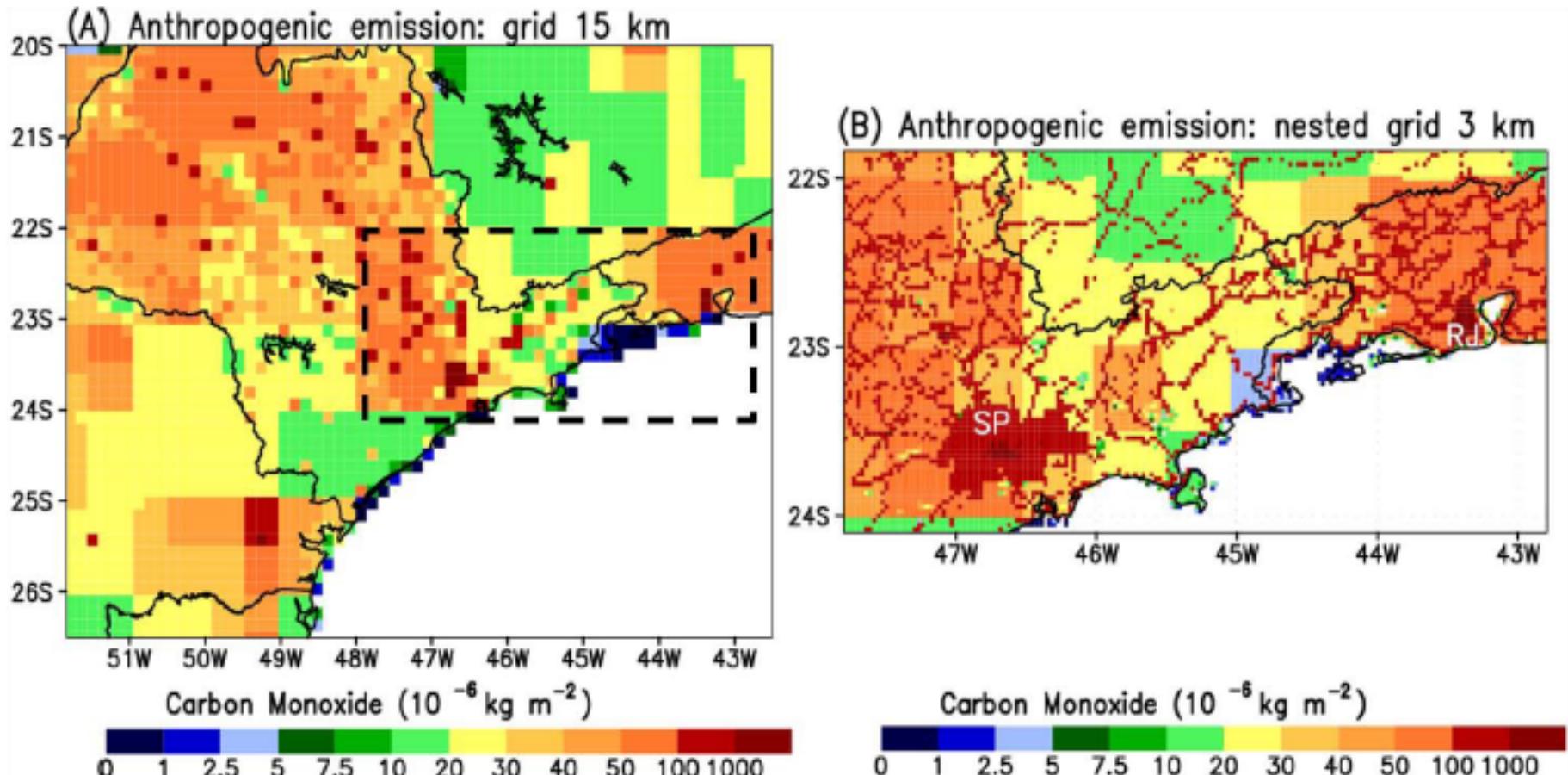
Anthropogenic emissions

Example for Alaska



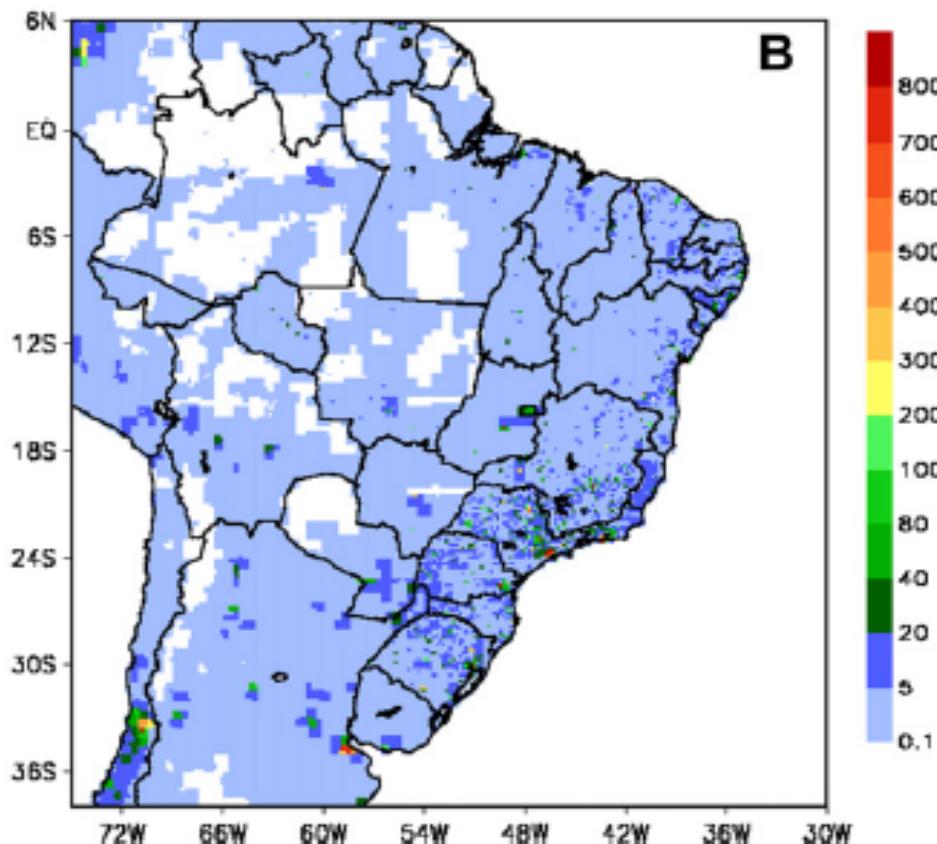
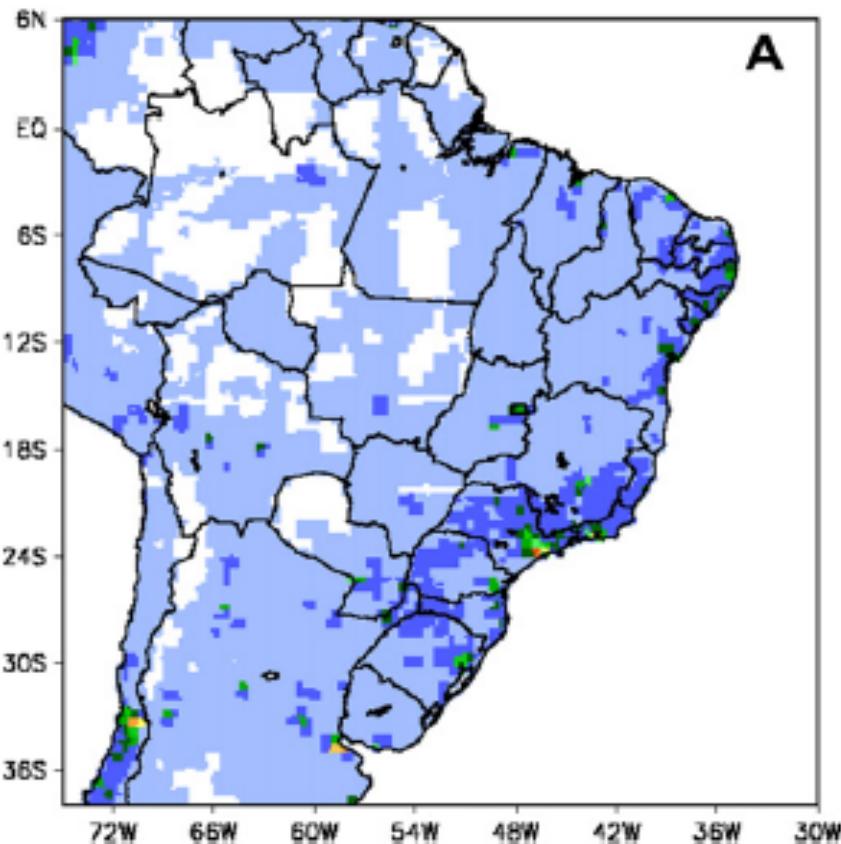
Anthropogenic emissions

AREA DELIMITER algorithm distributes emissions
on high resolution grids



Anthropogenic emissions

South America: Updated local inventories and extrapolation to cities without inventories based on socioeconomic data



CO emissions ($\times 10^6 \text{ kg m}^{-2} \text{ day}^{-1}$) on a 20 km grid covering South America without (A) and with (B) updated inventories

Biogenic emissions (bio_emiss_opt=0)

1) GEIA

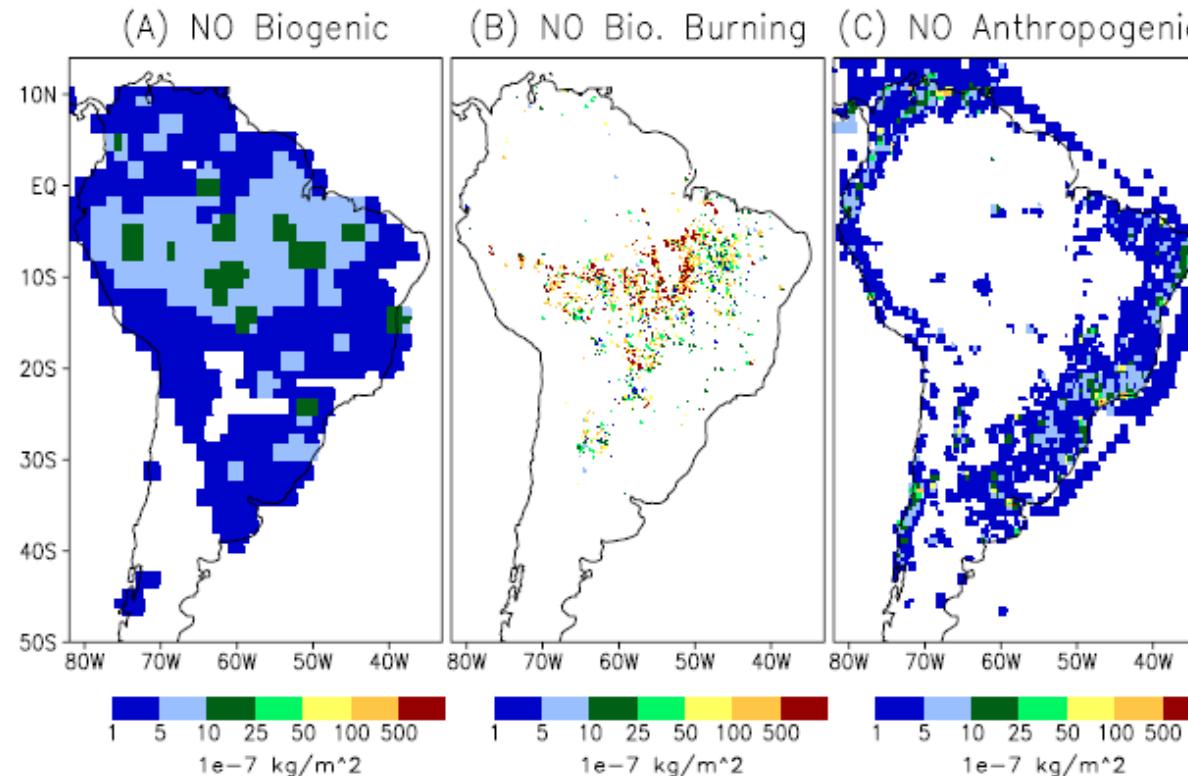
$1^{\circ} \times 1^{\circ}$, monthly, 2002

Acetone, C₂H₄, C₂H₆, C₃H₆,
C₃H₈, CO, CH₃OH, DMS, NO,
Isoprene, Terpenes and NVOC

2) MEGAN 2000 climatology

$0.5^{\circ} \times 0.5^{\circ}$, monthly, 2000

CO, CH₄, C₂H₄, C₂H₆, C₃H₆, C₃H₈,
CH₃OH, Formaldehyde, Acetaldehyde,
Acetone, other Ketones, Toluene,
Isoprene, Monoterpenes and
Sesquiterpenes



Daily emissions from (A) GEIA (B) 3BEM (C) RETRO for 27 August 2002 on a 0.2° grid

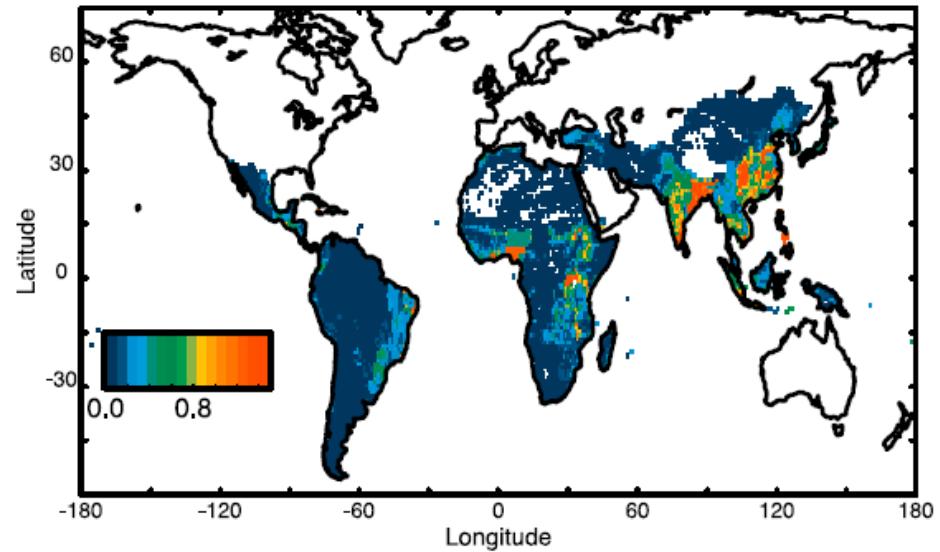
Alonso et al. (2010)

Biofuel burning in the developing world

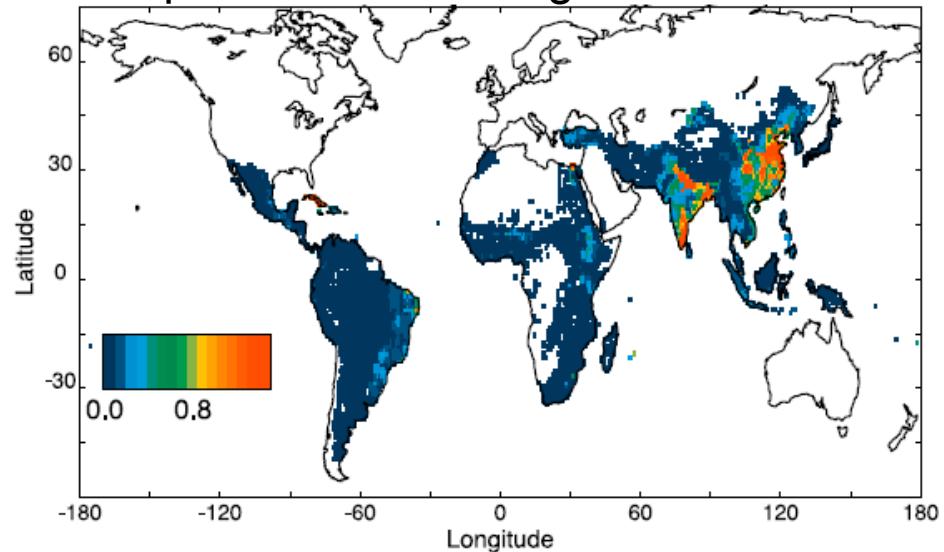
Emissions_Yevich_Logan

$1^0 \times 1^0$, Tg dry matter yr^{-1}

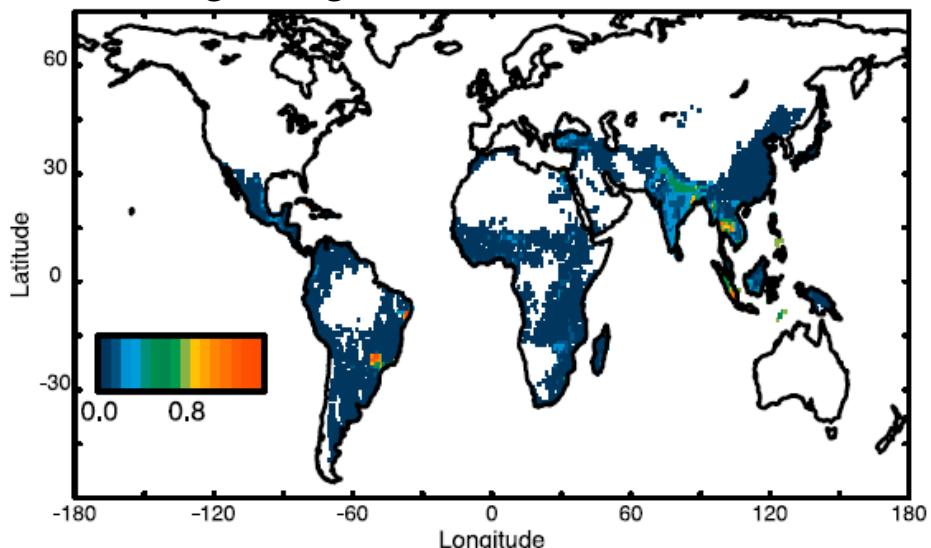
Woodfuel (fuelwood and charcoal) use



Crop residue and dung use

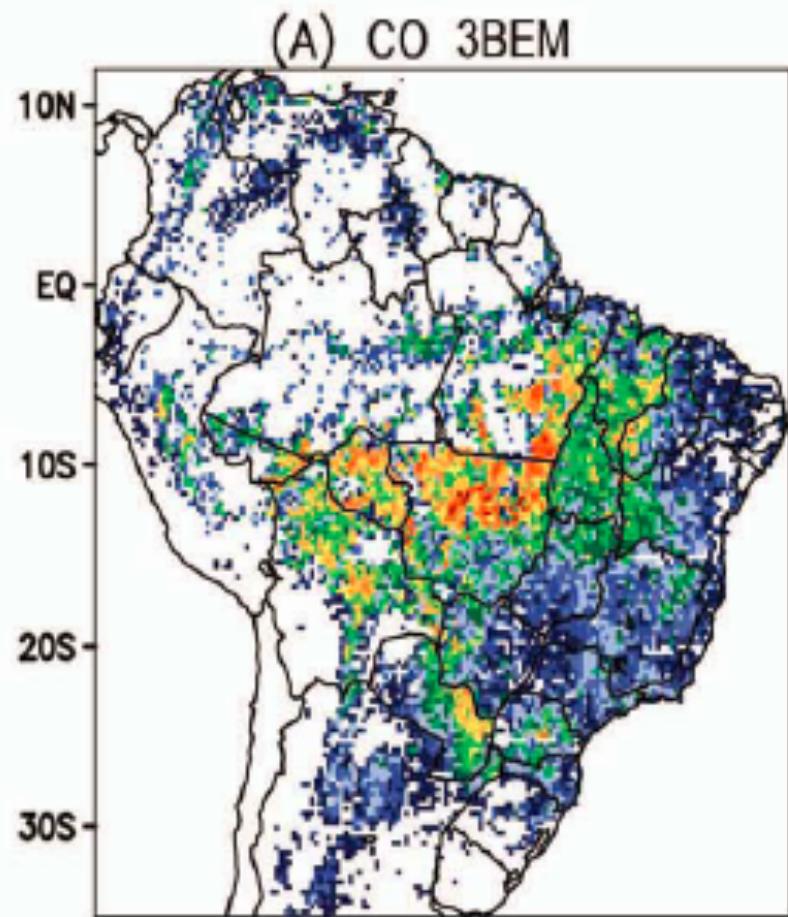


Burning of agricultural residue in the fields

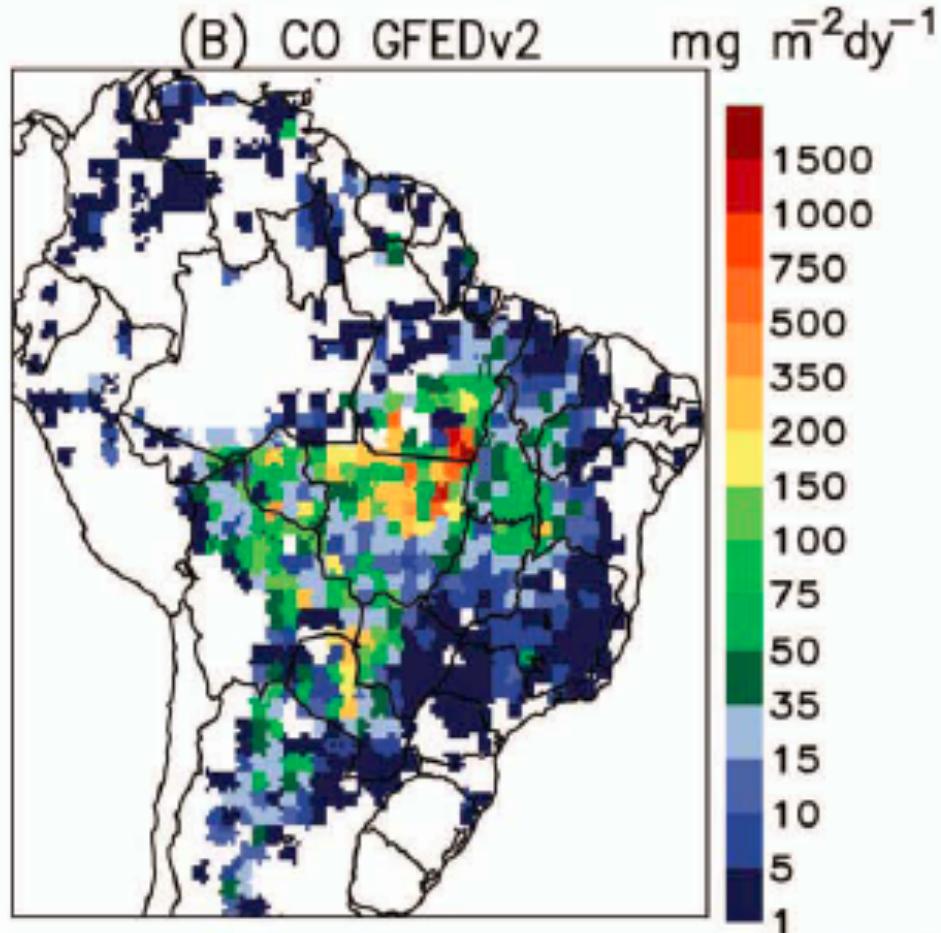


Biomass burning emissions

Brazilian Biomass Burning
Emission Model (**3BEM**)
Model resolution, daily



Global Fire Emissions Database (**GFEDv2**)
 $1^{\circ} \times 1^{\circ}$, 8-day or monthly, 1997 - 2004



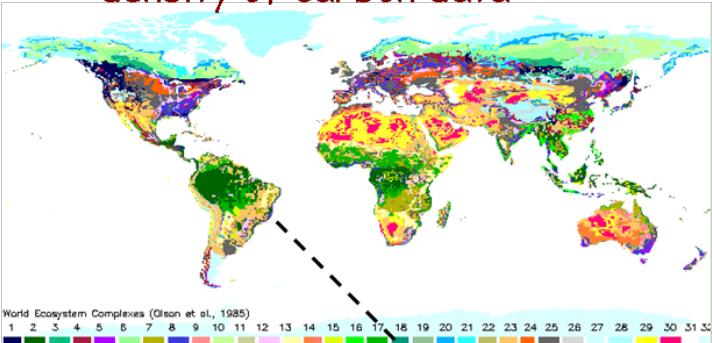
Average daily CO emissions, Aug.-Oct. 2002, 35 km

Freitas et al. (2011)

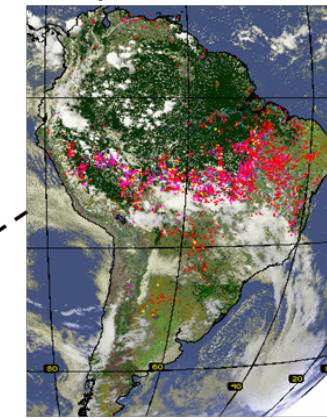
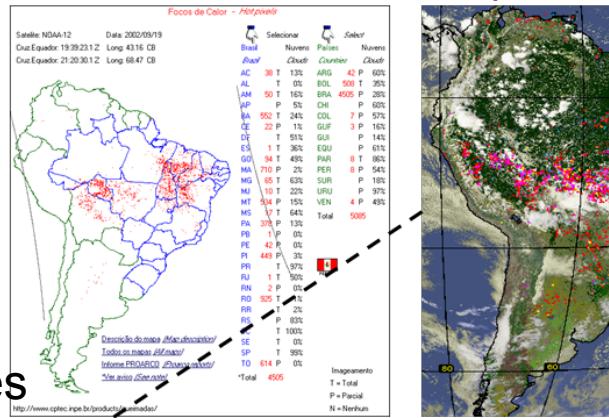
3BEM

Biomass burning emissions inventory Regional scale – daily basis

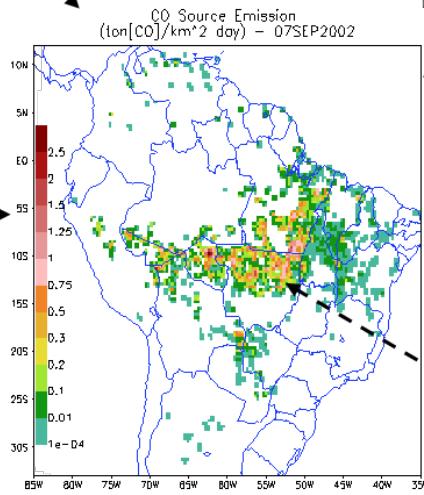
density of carbon data



near real time fire product



6 types of biomes 110 chemical species
land use data



CO source emission ($\text{kg m}^{-2}\text{day}^{-1}$)

Andreae and Merlet, 2001
emission & combustion factors

Biome category	Emission Factor for CO (g/kg)	Emission Factor for PM2.5 (g/kg)	Aboveground biomass density ($\alpha, \text{kg/m}^2$)	Combustion factor ($\beta, \text{fraction}$)
Tropical forest ¹	110.	8.3	20.7	0.48
South America savanna ²	63.	4.4	0.9	0.78
Pasture ³	49.	2.1	0.7	1.00

¹ Average values for primary and second-growth tropical forests, ² Average values for campo cerrado (C3) and cerrado sensu stricto (C4), ³ value for campo limpo (C1). All numbers are from Ward et al.,

mass estimation

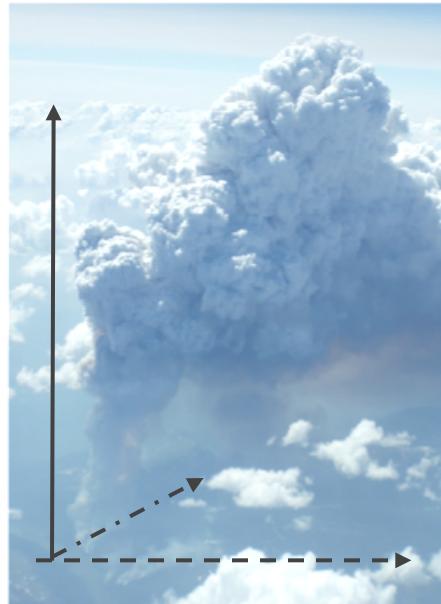
$$M_{[\eta]} = \alpha_{\text{veg}} \cdot \beta_{\text{veg}} \cdot E_f^{[\eta]} \cdot a_{\text{fire}},$$

3BEM Plume Rise

Biomass burning
and wildfires

Smoldering : mostly surface emission.

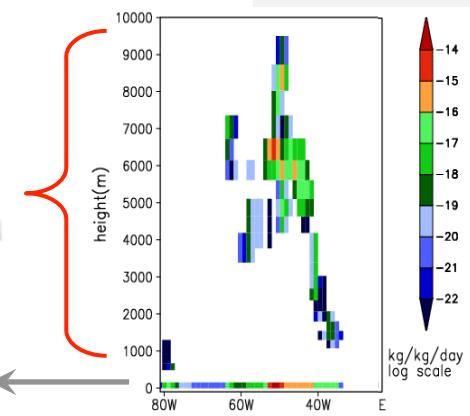
Flaming: mostly direct injection in the PBL,
free troposphere or stratosphere.



Example in
the model:

flaming
emission

smoldering
emission

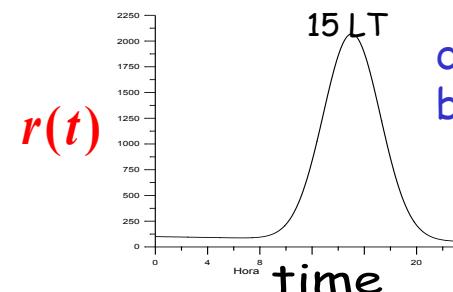
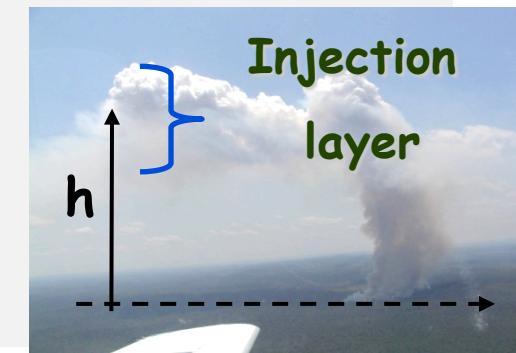


Plume rise model

total emission flux: F_η being λ the smoldering fraction

$$\text{smoldering term} : E_\eta = \frac{\lambda F_\eta}{\rho_{air} \Delta z_{\text{first phys. model layer}}}$$

$$\text{flaming term} : E_\eta = \frac{(1 - \lambda) F_\eta}{\rho_{air} \Delta z_{\text{injection layer}}}$$



diurnal cycle of the
burning for S. America:

$$E_\eta(t) = r(t) E_\eta$$

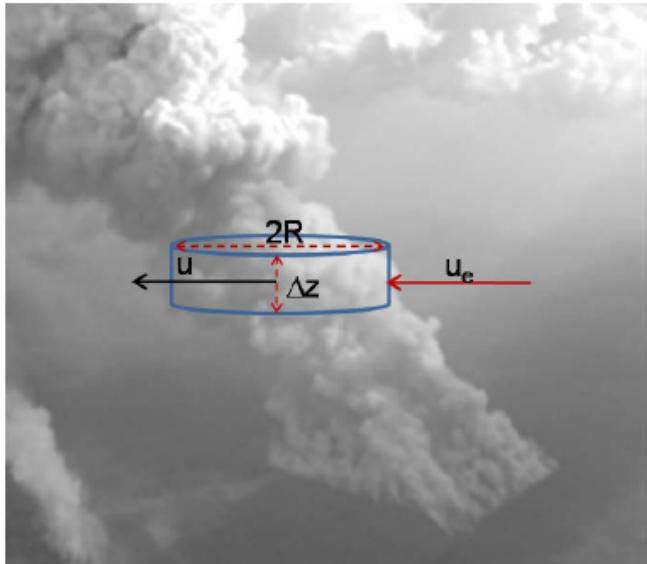
Freitas et al. (2011)

Environmental Wind Effects on Plume Rise



Biomass burning plumes in the Amazon region
without (left) and with (right) environmental wind shear
Photos: M.O. Andreae, M. Welling

Environmental Wind Effects on Plume Rise



$$\lambda_{\text{entr}} = \frac{2\alpha}{R} |w|$$

$$\delta_{\text{entr}} = \frac{2}{\pi R} (u_e - u)$$

W: vertical velocity

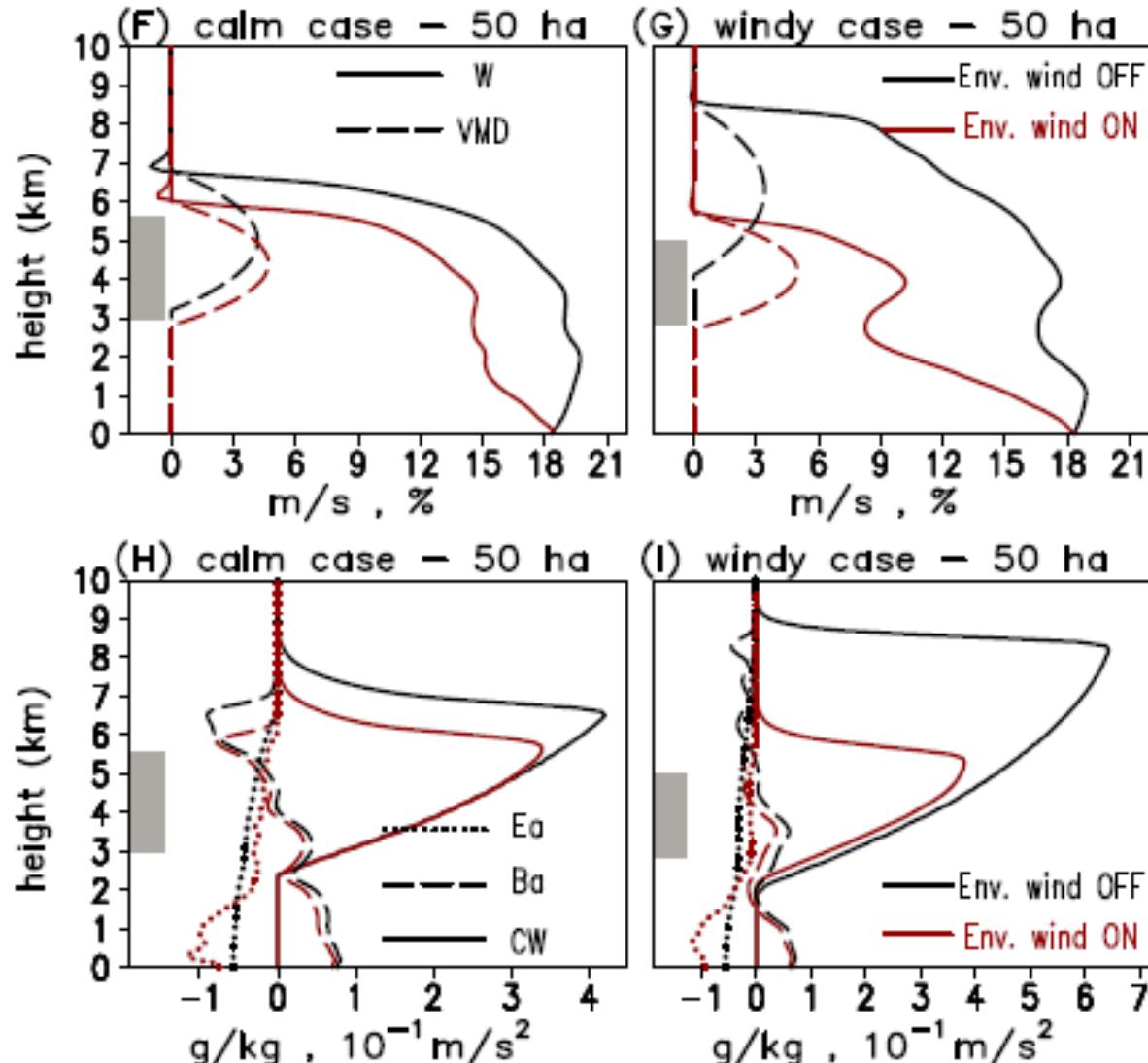
VMD: vertical mass distribution

Ea: Entrainment acceleration

Ba: buoyancy acceleration

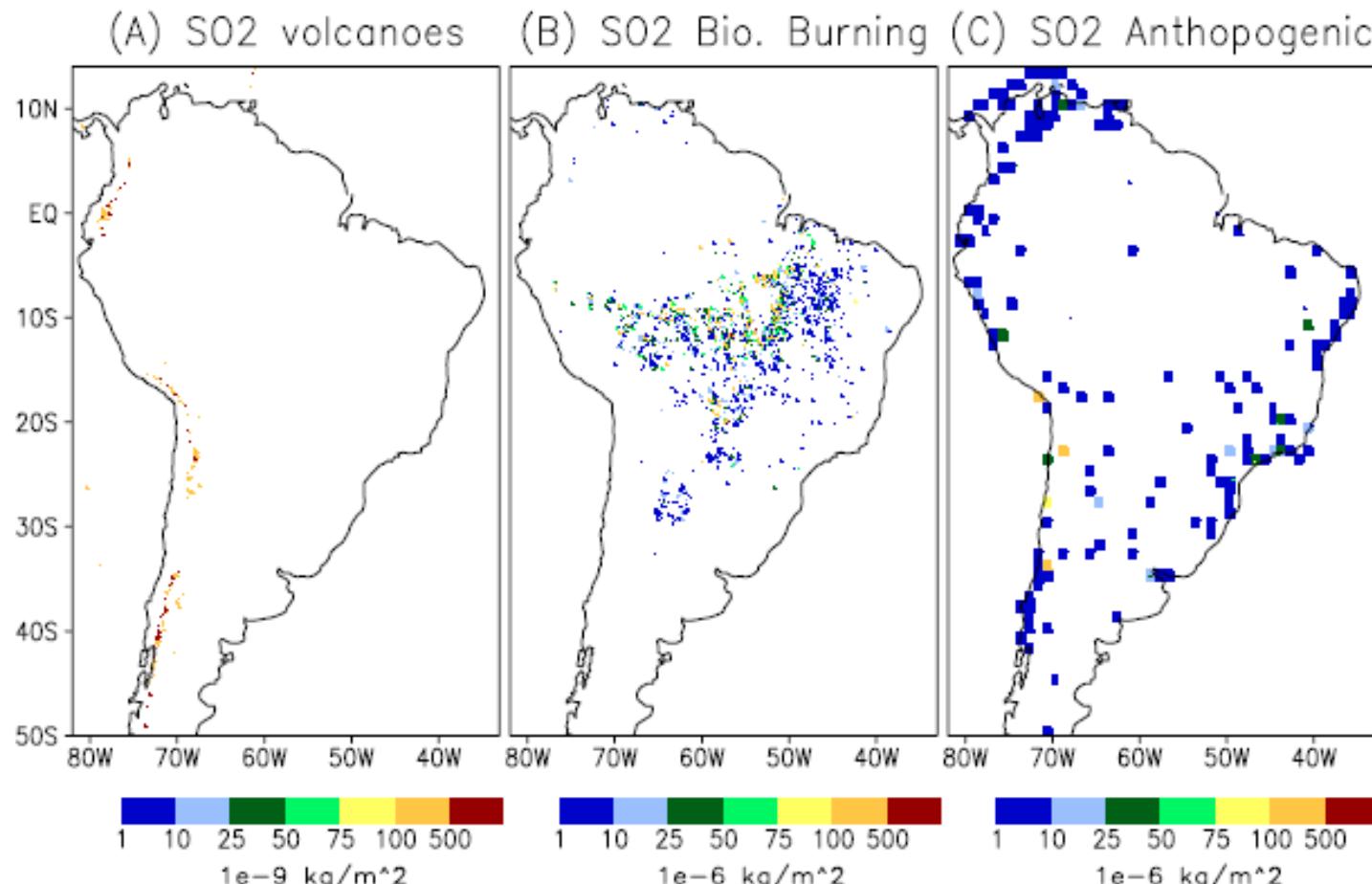
CW: total condensate water

1-D PRM results for a 50 ha fire,
calm and windy conditions



Volcano emissions

Based on Mastin et al. (2009) database of 1535 volcanoes
Mass eruption rate, plume height and time duration
SO₂ from AEROCOM program, 1979 – 2007 (Diehl, 2009)



SO₂ emissions on 27 August 2002 on a 0.2° rectangular projection
grid: (A) Diehl (2009), (B) 3BEM, (C) EDGAR

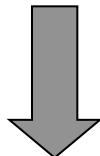
Freitas et al. (2011)

Compiling PREP-SRC-CHEM

Install libraries: netCDF, Zlib, HDF5

Set library paths in:

```
PREP-CHEM-SRC-1.x/bin/build/include.mk.<compiler>  
make OPT=<compiler>.wrf CHEM=RADM_WRF_FIM
```



Executable : *prep_chem_sources_RADM_WRF_FIM.exe*

Input file (namelist): *prep_chem_sources.inp*

Input file (namelist): prep_chem_sources.inp

```
$RP_INPUT
!----- grid_type
grid_type= 'lambert',          ! 'polar' = polar stereo. grid output
                                ! 'll'  = lat/lon grid output
                                ! 'lambert' = lambert grid output
                                ! 'mercator' = mercator grid output
!----- date of emission
ihour=0,
iday=12,
imon=7,
iyear=2004,
!----- select the sources datasets to be used: 1 = yes, 0 = not
use_retro=1,
retro_data_dir='/import/archive/u1/uaf/freitas/Emission_data/RETRO/anthro',
use_edgar =1, ! 0 - not, 1 - Version 3, 2 - Version 4 for some species
use_gocart=1,
user_data_dir='/home/poluicao/EMISSION_DATA/SouthAmerica_Megacities',
use_bioge =2, ! 1 - GEIA, 2 – MEGAN
use_fwbawb=1,
fwbawb_data_dir='/import/archive/u1/uaf/freitas/Emission_data/Emissions_Yevich_Logan',
use_gfedv2=0,
use_bbem=1,
use_bbem_plumerise=1,
```

Input file (namelist): prep_chem_sources.inp

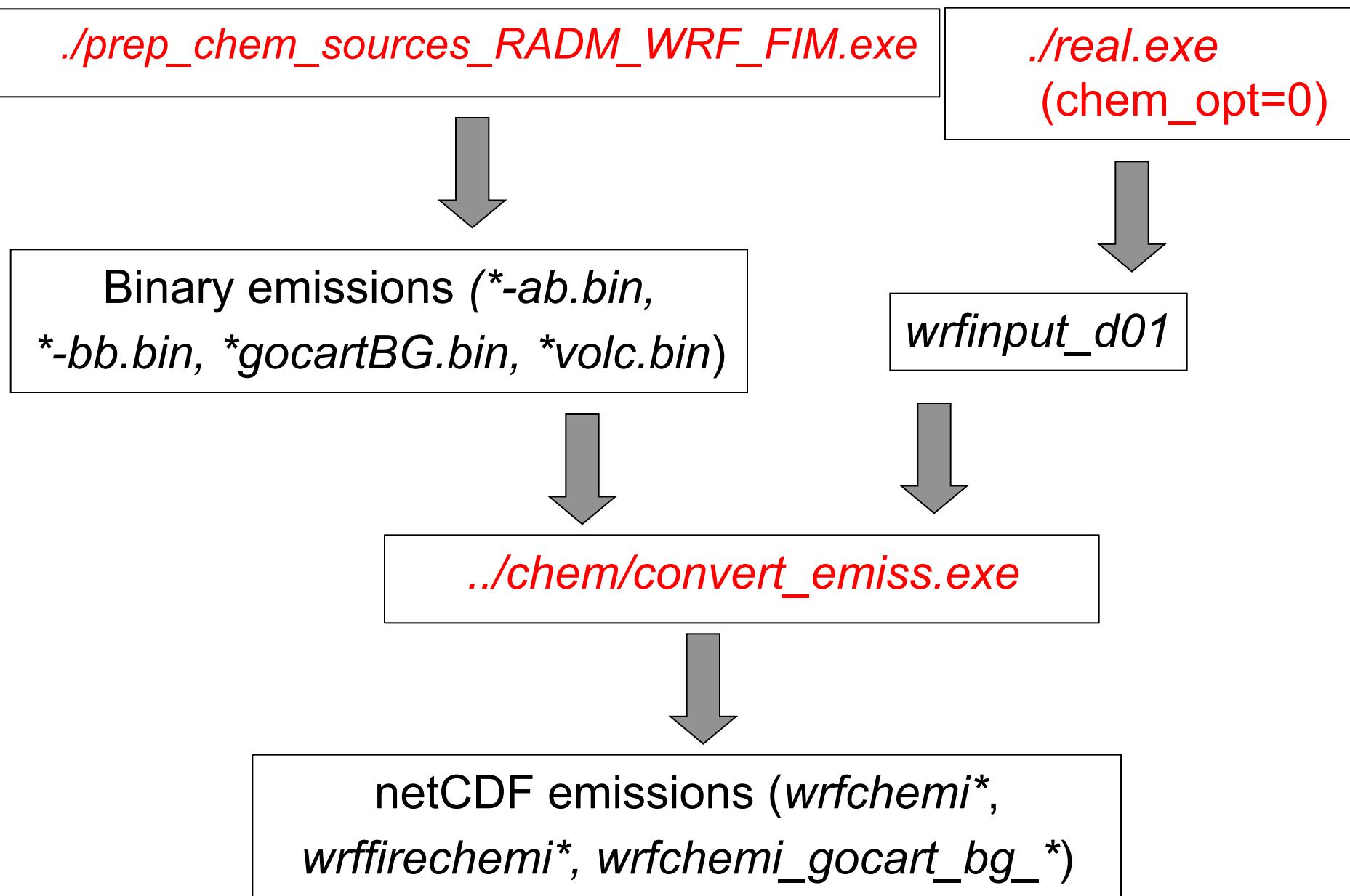
```
!----- if the merging of gfedv2 with bbem is desired (=1, yes, 0 = no)
merge_GFEDv2_bbem =0,  
  
!----- Fire product for 3BEM/3BEM-plumerise emission models
bbem_wfabba_data_dir='/import/archive/u1/uaf/freitas/Emission_data/fires_data/WF_ABBA/filt/f,
bbem_modis_data_dir  ='import/archive/u1/uaf/freitas/Emission_data/fires_data/MODIS/Fires.',
bbem_inpe_data_dir   ='import/archive/u1/uaf/freitas/Emission_data/fires_data/DSA/Focos',
bbem_extra_data_dir  ='import/archive/u1/uaf/freitas/Emission_data/fires_data/xxxxx,  
  
!----- gocart background
use_gocart_bg=1,  
!----- volcanoes emissions
use_volcanoes=0,
volcano_index=0, !REDOUBT
use_these_values='NONE',
! define a text file for using external values for INJ_HEIGHT, DURATION,
! MASS ASH (units are meters - seconds - kilograms) and the format for
! a file 'values.txt' is like this: 11000. 10800. 1.5e10
! use_these_values='values.txt',
begin_eruption='198912141930', !begin time UTC of eruption YYYYMMDDhhmm
!----- degassing volcanoes emissions
use_degass_volcanoes=0,
degass_volc_data_dir='/home/poluicao/EMISSION_DATA/VOLC_SO2',
```

Input file (namelist): prep_chem_sources.inp

!----- For regional grids (polar, Lambert, Mercator)

NGRIDS = 3, ! Number of grids to run
NNXP = 391,463,499, ! Number of x gridpoints
NNYP = 271,454,478, ! Number of y gridpoints
NXTNEST = 0, 1, 2, ! Grid number which is the next coarser grid
DELTAX = 18000,
DELTAY = 18000, ! X and Y grid spacing
! Nest ratios between this grid and the next coarser grid.
NSTRATX = 1, 3, 3, ! x-direction
NSTRATY = 1, 3, 3, ! y-direction
NINEST = 1, 78, 128, ! Grid point on the next coarser
NJNEST = 1, 30, 153, ! nest where the lower southwest
! NKNEST = 1, 1, 1, ! nest where the lower southwest
! corner of this nest will start.
! If NINEST or NJNEST = 0, use CENTLAT/LON
POLELAT = 15., ! If polar, latitude/longitude of pole point
POLELON = 10., ! If lambert, lat/lon of grid origin (x=y=0.)
STDLAT1 = 0., ! If polar, unused
STDLAT2 = 15., ! If lambert, standard latitudes of projection (truelat2/truelat1 from
namelist.wps, STDLAT1 < STDLAT2)
CENTLAT = 15.0,
CENTLON = 10.0,

Running PREP-CHEM-SRC and convert_emiss



References

- Alonso, M. F. ; Longo, K. M. ; Freitas, S. R. ; Fonseca, R. M. ; Marecal, V. ; Pirre, M. ; Gallardo, L. . An urban emissions inventory for South America and its application in numerical modeling of atmospheric chemical composition at local and regional scales. *Atmospheric Environment*, v. 44, p. 5072-5083, 2010.
- Freitas, S. R. ; Longo, K. M. ; Alonso, M. F. ; Pirre, M. ; Marecal, V. ; Grell, G. ; Stockler, R. ; Mello, R. F. ; Sánchez Gácita, M. . PREP-CHEM-SRC 1.0: a preprocessor of trace gas and aerosol emission fields for regional and global atmospheric chemistry models. *Geoscientific Model Development*, v. 4, p. 419-433, 2011.
- Freitas, S. R. , Longo, Karla , Trentmann, J. , Latham, D. Technical Note: Sensitivity of 1-D smoke plume rise models to the inclusion of environmental wind drag. *Atmospheric Chemistry and Physics*, v. 10, p. 585-594, 2010.
- Freitas, S. R., K. M. Longo, R. Chatfield, D. Latham, M. A. F. Silva Dias, M. O. Andreae, E. Prins, J. C. Santos, R. Gielow and J. A. Carvalho Jr.: Including the sub-grid scale plume rise of vegetation fires in low resolution atmospheric transport models. *Atmospheric Chemistry and Physics*, v. 7, p. 3385-3398, 2007.
- Freitas, S. R.; Longo, K. M.; M. Andreae. The impact of including the plume rise of vegetation fires in numerical simulations of associated atmospheric pollutants. *Geophys. Res. Lett.*, 33, L17808, doi:10.1029/2006GL026608, 2006.
- Yevich, R. and J.A. Logan, An assessment of biofuel use and burning of agricultural waste in the developing world, *Global Biogeochemical Cycles*, 2003

Thank you!

Questions?

gmai@cptec.inpe.br

megan.bela@colorado.edu